

# Splice Graphs and Their Topological Indices

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## Abstract

Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two graphs with disjoint vertex sets  $V_1$  and  $V_2$ . Let  $u_1 \in V_1$  and  $u_2 \in V_2$ . A splice of  $G_1$  and  $G_2$  by vertices  $u_1$  and  $u_2$ ,  $\mathcal{S}(G_1, G_2; u_1, u_2)$ , is defined by identifying the vertices  $u_1$  and  $u_2$  in the union of  $G_1$  and  $G_2$ . In this paper we calculate the Szeged, edge-Szeged,  $PI$ , vertex- $PI$  and eccentric connectivity indices of splice graphs.

## 1. Introduction

Let  $G = (V, E)$  be a simple graph with  $V$  and  $E$  being its vertex and edge sets, respectively. Graph theory has successfully provided chemists

with a variety of useful tools [2, 5], among which are the topological indices or molecular-graph-based structure descriptors [6, 7]. In this paper we are concerned with five of these topological indices, that recently attracted much attention and found noteworthy chemical applications.

All graphs considered in this paper are assumed to be simple, undirected, without weighted edges, and connected.

The **Szeged index** of a graph  $G$  is denoted by  $Sz(G)$  and defined as [8]

$$Sz = Sz(G) = \sum_{e=uv} n_u(e) n_v(e) . \quad (1)$$

Here the sum is taken over all edges of  $G$ , and for a given edge  $e = uv$ , the quantity  $n_u(e)$  denotes the number of vertices closer to  $u$  than to  $v$ , and the quantity  $n_v(e)$  is defined analogously. For more details on the Szeged index see the review [9] and the references cited therein.

Denote by  $d_G(x, y)$  the distance (= number of edges in a shortest path) between the vertices  $x$  and  $y$  of the graph  $G$ . Then we can define the sets

$$N(e, u, G) = \left\{ x \in V(G) \mid d_G(x, u) < d_G(x, v) \right\}$$

and

$$N(e, v, G) = \left\{ x \in V(G) \mid d_G(x, v) < d_G(x, u) \right\}$$

by means of which we have:

$$n_u(e) = n_u(e, G) = \left| N(e, u, G) \right| \quad \text{and} \quad n_v(e) = n_v(e, G) = \left| N(e, v, G) \right| .$$

It is obvious that an end-vertex of any edge is closer to itself than to the other end-vertex of that edge. Therefore the product  $n_u(e) n_v(e)$  is always positive.

The **edge-Szeged index** is obtained by replacing  $n_u(e) n_v(e)$  in Eq. (1) by  $m_u(e) m_v(e)$ , where  $m_u(e)$  is the number of edges in  $G$  whose distance to vertex  $u$  is smaller than the distance to vertex  $v$ , and  $m_v(e)$  is defined analogously. Hence the edge version of the Szeged index is given by [10]

$$Sz_e = Sz_e(G) = \sum_{e=uv} m_u(e) m_v(e) .$$

We recall that the distance between the edge  $f = xy$  and the vertex  $u$  in the graph  $G$ , denoted by  $d_G(f, u)$ , is define as  $d_G(f, u) = \min \left\{ d_G(x, u), d_G(y, u) \right\}$ . We can now introduce the sets

$$M(e, u, G) = \left\{ f \in E(G) \mid d_G(f, u) < d_G(f, v) \right\}$$

and

$$M(e, v, G) = \left\{ f \in E(G) \mid d_G(f, v) < d_G(f, u) \right\}$$

by means of which we have:

$$m_u(e) = m_u(e, G) = \left| M(e, u, G) \right| \quad \text{and} \quad m_v(e) = m_v(e, G) = \left| M(e, v, G) \right| .$$

If instead of multiplicative contributions  $n_u(e) n_v(e)$  and  $m_u(e) m_v(e)$ , we consider their additive versions,  $n_u(e) + n_v(e)$  and  $m_u(e) + m_v(e)$ , then we obtain the vertex- and the edge- $PI$  indices, respectively.<sup>1</sup>

The **edge-PI index** is defined as [11]

$$PI_e = PI_e(G) = \sum_{e=uv} \left[ m_u(e) + m_v(e) \right] .$$

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<sup>1</sup>The acronym  $PI$  comes from Padmakar and Ivan. Whereas Padmakar is the first name of P. V. Khadikar, the inventor of the  $PI$  index [11], Ivan comes from the first name of one of the present authors, whose contribution to the discovery of the  $PI$  index was nil.

Since this edge version was introduced first, the subscript  $e$  is usually omitted and the index is referred to simply as  $PI$  index. More details on the  $PI$  index are found in the review [12] and the references cited therein.

The **vertex-PI index** seems to have first been considered by Khalifeh et al. [13] and is defined as

$$PI_v = PI_v(G) = \sum_{e=uv} [n_u(e) + n_v(e)] .$$

The **eccentric connectivity index** of the graph  $G$  is defined as [15]

$$Ecc = Ecc(G) = \sum_{u \in V} \deg(u) \varepsilon(u) \quad (2)$$

where for a given vertex  $u$ , its eccentricity  $\varepsilon(u)$  is the greatest distance between  $u$  and any other vertex of  $G$ . The maximum eccentricity over all vertices of  $G$  is called the *diameter* of  $G$  whereas the minimum eccentricity among the vertices of  $G$  is the *radius* of  $G$ . The set of vertices whose eccentricity is equal to the radius of  $G$  is called the *center* of  $G$ . It is well known that each tree has either one or two vertices in its center.

The aim of this article is to contribute to the theory of the above described five topological indices by showing how these can be computed in the case of splice graphs.

Suppose that  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  are two graphs with disjoint vertex sets. Let  $u_1 \in V_1$  and  $u_2 \in V_2$  be given vertices of  $G_1$  and  $G_2$ , respectively. Following Došlić [4], a splice of  $G_1$  and  $G_2$  by vertices  $u_1$  and  $u_2$ ,  $\mathcal{S}(G_1, G_2; u_1, u_2)$ , is defined by identifying the vertices  $u_1$  and  $u_2$  in the union of  $G_1$  and  $G_2$  (See Figure 1).

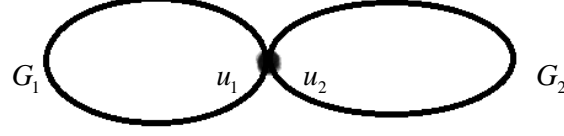


Figure 1: The splice graph  $\mathcal{S}(G_1, G_2; u_1, u_2)$  and the labeling of its structural details.

Some topological indices of splice graphs are computed already [1, 3, 14, 16]. In this paper we aim to compute some other indices for these graphs. Note that the idea of the proofs is based on that of a previously communicated work [17].

## 2. Main Results

In this section, we compute the Szeged, edge-Szeged, edge- $PI$ , vertex- $PI$ , and eccentric connectivity indices of the above described splice graph. We first introduce the following structural parameters of  $\mathcal{S} = \mathcal{S}(G_1, G_2; u_1, u_2)$ . Let  $i = 1, 2$  and  $f = xy \in E_i$ , and

$$\begin{aligned} n_x^i(f) &= |N(f, x, G_i)| & , & \quad n_y^i(f) = |N(f, y, G_i)| \\ n_x(f) &= |N(f, x, \mathcal{S})| & , & \quad n_y(f) = |N(f, y, \mathcal{S})| \\ m_x^i(f) &= |M(f, x, G_i)| & , & \quad m_y^i(f) = |M(f, y, G_i)| \\ m_x(f) &= |M(f, x, \mathcal{S})| & , & \quad m_y(f) = |M(f, y, \mathcal{S})| . \end{aligned}$$

In addition, for a given vertex  $u \in V(\mathcal{S})$ , let  $\varepsilon_1(u)$  be the eccentricity of  $u$  as a vertex of  $G_1$ ,  $\varepsilon_2(u)$  the eccentricity of  $u$  as a vertex of  $G_2$ , and  $\varepsilon(u)$  the eccentricity of  $u$  as a vertex of the splice graph  $\mathcal{S}$ .

**Proposition 1.** *Assume that  $f = xy \in E_1$ .*

(i) *If  $u_1 \in N(f, x, G_1)$ , then*

$$\begin{aligned} n_x(f) &= n_x^1(f) + |V_2| \quad , \quad n_y(f) = n_y^1(f) \\ m_x(f) &= m_x^1(f) + |E_2| \quad , \quad m_y(f) = m_y^1(f) . \end{aligned}$$

(ii) *If  $d_{G_1}(u_1, x) = d_{G_1}(u_1, y)$ , then*

$$\begin{aligned} n_x(f) &= n_x^1(f) \quad , \quad n_y(f) = n_y^1(f) \\ m_x(f) &= m_x^1(f) \quad , \quad m_y(f) = m_y^1(f) . \end{aligned}$$

*Analogous relations hold if  $f = xy \in E_2$ .*

*Proof* is easy and is left to the reader.

In order to verify the following propositions we need some preparations.

For  $i = 1, 2$ , let

$$S_i = \left\{ f = xy \in E_i \mid d_{G_i}(x, u_i) = d_{G_i}(y, u_i) \right\} \quad , \quad T_i = E_i \setminus S_i \quad , \quad t_i = |T_i| .$$

In addition, for  $f = xy \in E_i$  define

$$n^i(f) = \begin{cases} n_x^i(f) & \text{if } d_{G_i}(x, u_i) > d_{G_i}(y, u_i) \\ n_y^i(f) & \text{if } d_{G_i}(x, u_i) < d_{G_i}(y, u_i) \\ 0 & \text{if } d_{G_i}(x, u_i) = d_{G_i}(y, u_i) \end{cases}$$

and

$$m^i(f) = \begin{cases} m_x^i(f) & \text{if } d_{G_i}(x, u_i) > d_{G_i}(y, u_i) \\ m_y^i(f) & \text{if } d_{G_i}(x, u_i) < d_{G_i}(y, u_i) \\ 0 & \text{if } d_{G_i}(x, u_i) = d_{G_i}(y, u_i) . \end{cases}$$

**Proposition 2.**

$$\begin{aligned}
Sz(\mathcal{S}) &= Sz(G_1) + Sz(G_2) \\
&+ |V_2| \sum_{f=xy \in E_1} n^1(f) + |V_1| \sum_{f=xy \in E_2} n^2(f) .
\end{aligned}$$

*Proof.*

$$\begin{aligned}
Sz(\mathcal{S}) &= \sum_{f=xy \in E_1} n_x(f) n_y(f) + \sum_{f=xy \in E_2} n_x(f) n_y(f) \\
&= \sum_{f=xy \in E_1} n_x^1(f) n_y^1(f) + \sum_{f=xy \in E_1} |V_2| n^1(f) \\
&+ \sum_{f=xy \in E_2} n_x^2(f) n_y^2(f) + \sum_{f=xy \in E_2} |V_1| n^2(f) . \tag{3}
\end{aligned}$$

Because for  $i = 1, 2$ ,

$$\sum_{f=xy \in E_i} n_x^i(f) n_y^i(f) = Sz(G_i)$$

from Eq. (3) we directly obtain Proposition 2. □

**Proposition 3.**

$$\begin{aligned}
Sz_e(\mathcal{S}) &= Sz_e(G_1) + Sz_e(G_2) \\
&+ |E_2| \sum_{f=xy \in E_1} m^1(f) + |E_1| \sum_{f=xy \in E_2} m^2(f) .
\end{aligned}$$

*Proof.*

$$Sz_e(\mathcal{S}) = \sum_{f=xy \in E_1} m_x(f) m_y(f) + \sum_{f=xy \in E_2} m_x(f) m_y(f)$$

$$\begin{aligned}
&= \sum_{f=xy \in E_1} m_x^1(f) m_y^1(f) + \sum_{f=xy \in E_1} |E_2| m^1(f) \\
&+ \sum_{f=xy \in E_2} m_x^2(f) m_y^2(f) + \sum_{f=xy \in E_2} |E_1| m^2(f) . \tag{4}
\end{aligned}$$

Because for  $i = 1, 2$ ,

$$\sum_{f=xy \in E_i} m_x^i(f) m_y^i(f) = Sz_e(G_i)$$

from Eq. (4) we directly obtain Proposition 3. □

**Proposition 4.**

$$PI_v(\mathcal{S}) = PI_v(G_1) + PI_v(G_2) + (t_2 + 1)|V_1| + (t_1 + 1)|V_2| .$$

*Proof.*

$$\begin{aligned}
PI_v(\mathcal{S}) &= \sum_{f=xy \in T_1} [n_x(f) + n_y(f)] + \sum_{f=xy \in S_1} [n_x(f) + n_y(f)] \\
&+ \sum_{f=xy \in T_2} [n_x(f) + n_y(f)] + \sum_{f=xy \in S_2} [n_x(f) + n_y(f)] + [n_{u_1}(e) + n_{u_2}(e)] \\
&= \sum_{f=xy \in T_1} [n_x^1(f) + |V_2| + n_y^1(f)] + \sum_{f=xy \in S_1} [n_x^1(f) + n_y^1(f)] \\
&+ \sum_{f=xy \in T_2} [n_x^2(f) + |V_1| + n_y^2(f)] + \sum_{f=xy \in S_2} [n_x^2(f) + n_y^2(f)] + (|V_1| + |V_2|) \\
&= \sum_{f=xy \in T_1} [n_x^1(f) + n_y^1(f)] + t_1 |V_2| + \sum_{f=xy \in S_1} [n_x^1(f) + n_y^1(f)] \\
&+ \sum_{f=xy \in T_2} [n_x^2(f) + n_y^2(f)] + t_2 |V_1| + \sum_{f=xy \in S_2} [n_x^2(f) + n_y^2(f)] \\
&+ (|V_1| + |V_2|) . \tag{5}
\end{aligned}$$



Because for  $i = 1, 2$ ,

$$\sum_{f=xy \in T_i} [n_x^i(f) + n_y^i(f)] + \sum_{f=xy \in S_i} [n_x^i(f) + n_y^i(f)] = \sum_{f=xy \in E_i} [n_x^i(f) + n_y^i(f)] = PI_v(G_i)$$

from Eq. (5) we directly obtain Proposition 4.  $\square$

**Proposition 5.**

$$PI(\mathcal{S}) = PI(G_1) + PI(G_2) + t_2|E_1| + t_1|E_2| .$$

*Proof.*

$$\begin{aligned} PI(\mathcal{S}) &= \sum_{f=xy \in T_1} [m_x(f) + m_y(f)] + \sum_{f=xy \in S_1} [m_x(f) + m_y(f)] \\ &+ \sum_{f=xy \in T_2} [m_x(f) + m_y(f)] + \sum_{f=xy \in S_2} [m_x(f) + m_y(f)] + [m_{u_1}(e) + m_{u_2}(e)] \\ &= \sum_{f=xy \in T_1} [m_x^1(f) + |E_2| + m_y^1(f)] + \sum_{f=xy \in S_1} [m_x^1(f) + m_y^1(f)] \\ &+ \sum_{f=xy \in T_2} [m_x^2(f) + |E_1| + m_y^2(f)] + \sum_{f=xy \in S_2} [m_x^2(f) + m_y^2(f)] \\ &= \sum_{f=xy \in T_1} [m_x^1(f) + m_y^1(f)] + t_1|E_2| + \sum_{f=xy \in S_1} [m_x^1(f) + m_y^1(f)] \\ &+ \sum_{f=xy \in T_2} [m_x^2(f) + m_y^2(f)] + t_2|E_1| + \sum_{f=xy \in S_2} [m_x^2(f) + m_y^2(f)] . \end{aligned}$$

Because for  $i = 1, 2$ ,

$$\sum_{f=xy \in T_i} [m_x^i(f) + m_y^i(f)] + \sum_{f=xy \in S_i} [m_x^i(f) + m_y^i(f)] = \sum_{f=xy \in E_i} [m_x^i(f) + m_y^i(f)] = PI(G_i)$$

from Eq. (6) we directly obtain Proposition 5.  $\square$

**Proposition 6.**

$$\begin{aligned}
Ecc(\mathcal{S}) &= \sum_{x \in V_1} \deg_{\mathcal{S}}(x) \cdot \max \left\{ d_{G_1}(x, u_1) + \varepsilon_2(u_2), \varepsilon_1(x) \right\} \\
&+ \sum_{y \in V_2} \deg_{\mathcal{S}}(y) \cdot \max \left\{ d_{G_2}(y, u_2) + \varepsilon_1(u_1), \varepsilon_2(y) \right\}.
\end{aligned}$$

*Proof.* Consider a vertex  $x$  of the splice graph  $\mathcal{S}$ , such that  $x \in V_1$ . Let  $z$  be the vertex of  $\mathcal{S}$  whose distance to  $x$  is maximal. Thus,  $\varepsilon(x) = d_{\mathcal{S}}(x, z)$ . If  $z$  belongs to the graph  $G_1$ , then  $\varepsilon(x) = \varepsilon_1(x)$ . If  $z$  belongs to the graph  $G_2$ , then the distance between  $x$  and  $z$  is equal to  $d_{G_1}(x, u_1) + d_{G_2}(u_2, z)$ , see Fig. 1. In addition,  $z$  must be the vertex at greatest distance from  $u_2$ . Consequently,  $\varepsilon(x) = d_{G_1}(x, u_1) + \varepsilon_2(u_2)$ . This means that no matter where the vertex  $z$  is located,

$$\varepsilon(x) = \max \left\{ d_{G_1}(x, u_1) + \varepsilon_2(u_2), \varepsilon_1(x) \right\}$$

holds for any vertex  $x \in V_1$ . The formula for  $\varepsilon(y)$  in the case when  $y \in V_2$  is fully analogous.

Proposition 6 follows now from the definition of the eccentric connectivity index, Eq. (2). □

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